A 2-D Model to Simulate Convection and Phase Transitions Accurately

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An accurate modeling of phase change interfaces during solidifying flows has very relevant applications to materials science and metallurgical processes. For example, castings of metal alloys can experience undesirable macrosegregation, which reduces strength and quality control. However, monitoring solidification processes is difficult to achieve experimentally, so state-of-the-art mathematical models of this effect are crucial. Simulations of phase change convection include significant nonlinear processes such as the release of latent heat and the deceleration of natural convection in the melt that must be resolved in time to achieve accurate solutions.

We have developed a two-dimensional (2-D) phase change model with convection using the incompressible Navier-Stokes equation set and enthalpy as the energy conservation variable. An enthalpy framework allows latent heat changes to be tracked explicitly rather than extracting an approximate phase front from the final temperature field [1]. The equation set can be solved with the popular SIMPLE pressure correction algorithm, whereby the equation set is solved sequentially. It is well known that the SIMPLE family of solvers converges easily but relatively slowly for phase change problems. To improve accuracy and efficiency, we have implemented the Jacobian-Free Newton-Krylov (JFNK) solution method with SIMPLE as a preconditioner. JFNK solves fully coupled nonlinear equation sets and has been applied successfully to a range of nonlinear applications ([2] provides a good review). Applying several sweeps of SIMPLE provides an approximate update for the main algorithm.

To assess the accuracy and efficacy of the JFNK-SIMPLE algorithm for convection phase change applications, we simulate the freezing of a nondimensional pure material in a benchmark 2-D square cavity with a domain configuration matching earlier studies. This freezing simulation is run for a set of varying time step sizes. As the time step increases, the number of nonlinear iterations required to converge remains relatively constant. The solver shifts the work of iterating to solution to the faster inner linear algorithm, which maximizes convergence speed. The same simulation is also run using the SIMPLE algorithm as the main solver, and it is about 4 times slower on a 50^2 grid for the same time step. For a 200^2 grid, SIMPLE cannot run to convergence above 0.001 s time step, whereas JFNK-SIMPLE can run at 0.2 s. At these time steps, JFNK-SIMPLE is 200 times faster.

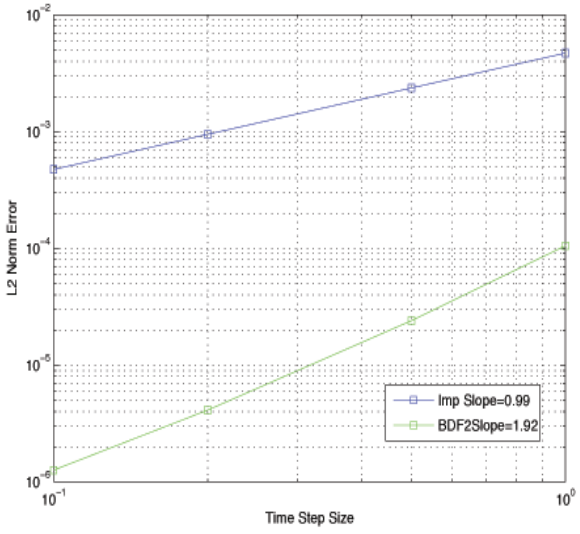

Fig. 1.
Time step convergence for nondimensional freezing within a cavity of natural convection. The blue and green lines indicate the L_2 norm of error for simulations with first- and second-order discretization respectively. The slopes indicate that the algorithm achieves first- and second-order convergence.

The other crucial measure of algorithm performance is accuracy, which is assessed by comparing simulations to a base run with a time step size of $1x10^{-3}$ s using BDF2 second-order time discretization. Error is

measured with a global L_2 time discretizations as a function of time step is presented in Fig. 1. The slope of the line of error vs time step size on a log-log plot provides the order of accuracy. The slope of the first-order runs is 0.99 and BDF2 is 1.92 over an order of magnitude of time step sizes, which demonstrates first- and second-order accurate solutions.

The JFNK-SIMPLE algorithm is also applied to a gallium (Ga) melting problem. For consistency, the domain configuration is set to match a portion of Gau and Vistanka's [3] experimental set-up and several earlier Ga melting simulations. This simulation was run for 200 s and the resulting streamfunction contours in the melt are displayed every 40 s in Fig. 2. The Ga melting problem is significantly more complex than nondimensional freezing because early in the melting simulation, the aspect ratio of the melted region is very high. As a result, instabilities in the convection melt induce multiple roll cell structure that significantly influences the structure of the phase front and requires a highly accurate solution method to resolve. Note the undulations of the phase front (denoted by the red line) along the vertical axis in Fig. 2. Like the freezing problem, using the JFNK-SIMPLE algorithm allows the Ga melting problem to be run at time steps 200 greater than with SIMPLE. Thus, it can run to completion 41.5 times faster to the same nonlinear tolerance.

For both freezing and melting simulations of 2-D phase change convection, the JFNK algorithm preconditioned with SIMPLE provides quantifiably low error with superior efficiency. With this algorithmic tool, the conditions and time scales within which multiple cell structure develops during phase change convection can be studied in more detail.

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[1] D.A. Knoll, et al., *Num. Heat Trans. B* **35**, 439–459 (1999).
[2] D.A. Knoll and D. Keyes, *J. Comput. Phys.* **193,** 357–397 (2004).
[3] C. Gau and R. Vistanka, *J. Heat Trans.* **108,** 171–174 (1986).

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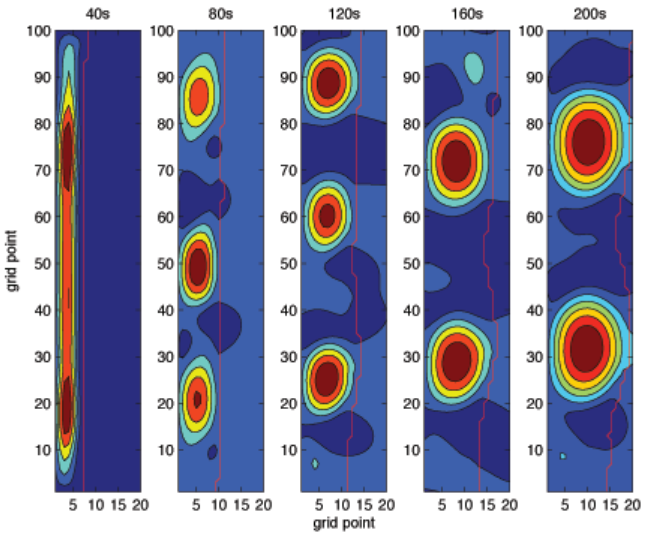

Fig. 2.
Melting and convection of pure Ga displayed for the 40x100 grid every 40 s. The contours are values of stream-function. The red line denotes the fully frozen contour.